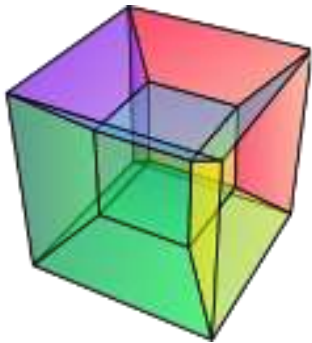


HyperSpy Community & Github

Eric Prestat

University of Manchester and SuperSTEM Laboratory



- HyperSpy on the web
- What is Github? Why is it so popular?
- What makes the HyperSpy community?



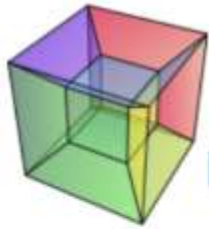
'Enhanced Data Generated by Electrons'

Following the very successful workshops at Lake Tahoe, Leukerbad, Port Ludlow, Guadeloupe, Grundlsee and Banff, the next international workshop on electron energy loss spectroscopy and imaging will be held in

Sainte Maxime, France,

- Francisco's talk on HyperSpy
 - Mostly about open source and scientific python community
 - NOT about the cool stuff that HyperSpy could already do at the time
- Open source **is not only** about opening the source code, it is also about:
 - Accessibility to the users
 - Sustainable library development
 - Building a community





HyperSpy

multi-dimensional data analysis

[Home](#) · [Download](#) · [Documentation](#) · [Demos](#) · [News](#) · [Support](#) · [Citing](#) · [Credits](#)

HyperSpy: multi-dimensional data analysis toolbox

HyperSpy is an open source Python library which provides tools to facilitate the interactive data analysis of multi-dimensional datasets that can be described as multi-dimensional arrays of a given signal (e.g. a 2D array of spectra a.k.a spectrum image).

HyperSpy aims at making it easy and natural to apply analytical procedures that operate on an individual signal to multi-dimensional arrays, as well as providing easy access to analytical tools that exploit the multi-dimensionality of the dataset.

Its modular structure makes it easy to add features to analyze different kinds of signals.

Highlights

- Two families of named and scaled axes: *signal* and *navigation*.
- Visualization tools for multi-dimensional spectra and images.
- Easy access multi-dimensional curve fitting and blind source separation.
- Built on top of NumPy, SciPy, matplotlib and scikit-learn.
- Modular design for easy extensibility.

HyperSpy documentation/community support

- Main website:
 - <https://hyperspy.org/>
- Documentation:
 - <https://hyperspy.org/hyperspy-doc/current/index.html>
- Gitter: online chat room
 - <https://gitter.im/hyperspy/hyperspy>
- Users list:
 - <https://groups.google.com/forum/#!forum/hyperspy-users>
 - Not used much anymore in favour of gitter

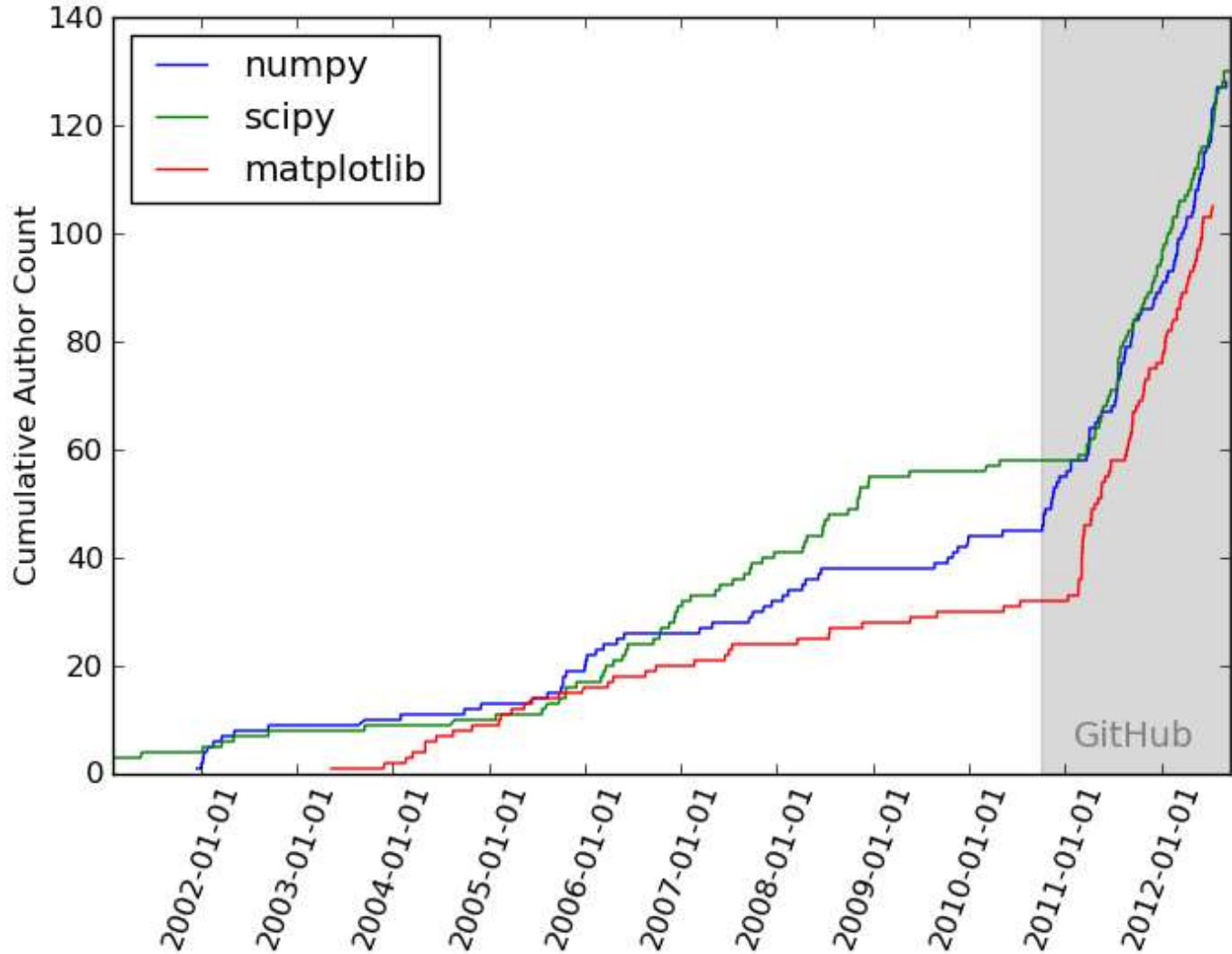
HyperSpy demos

- Source code of the demo on github
 - <https://github.com/hyperspy/hyperspy-demos>
- Non-interactive version on [nbviewer](https://nbviewer.jupyter.org/github/hyperspy/hyperspy-demos/tree/master/)
 - <https://nbviewer.jupyter.org/github/hyperspy/hyperspy-demos/tree/master/>
 - Github now displays nicely the notebook, but works well for short notebook (loading fail otherwise)
- Interactive version on mybinder.org
 - <https://mybinder.org/v2/gh/hyperspy/hyperspy-demos/master>
 - Run demos online (on a remote server) without any installation
 - 1 CPU core, between 1 and 2 GB available memory
 - Shut down after 10 min inactivity

HyperSpy development

- Development site on Github
 - <https://github.com/hyperspy/hyperspy>
 - Issues tracker: report bug, propose new features and other business
 - Pull requests: discuss the merge of any changes with the upstream branches
- Developer guide
 - http://hyperspy.readthedocs.io/en/stable/dev_guide.html

The github effect



From Pythonic perambulations: Why Python is the last language you'll have to learn:

<https://jakevdp.github.io/blog/2012/09/20/why-python-is-the-last/>

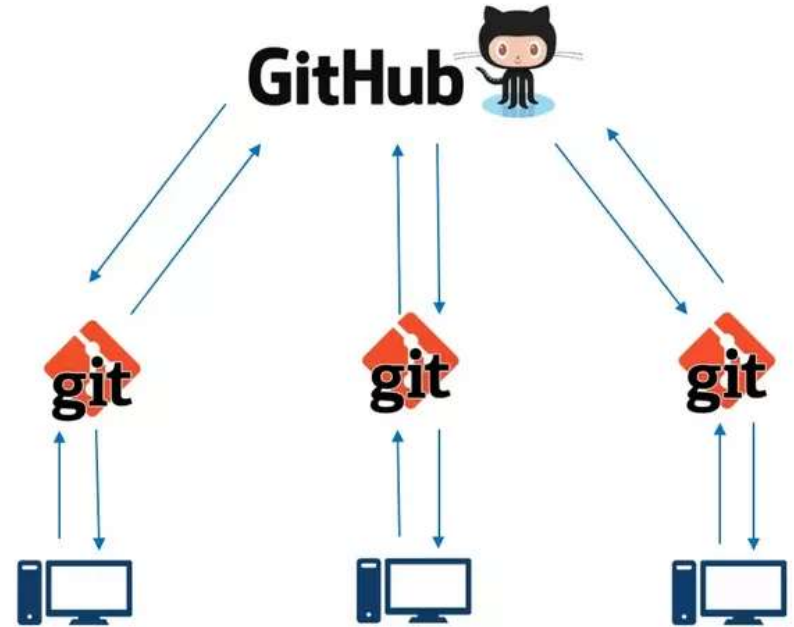
What is github?

- At the heart of Github is **git**
 - A version control system: manages and stores revisions of projects
 - git is a distributed version control systems
 - Each contributor has is own *remote* (online) repository
 - Code is merged in the *upstream* repository

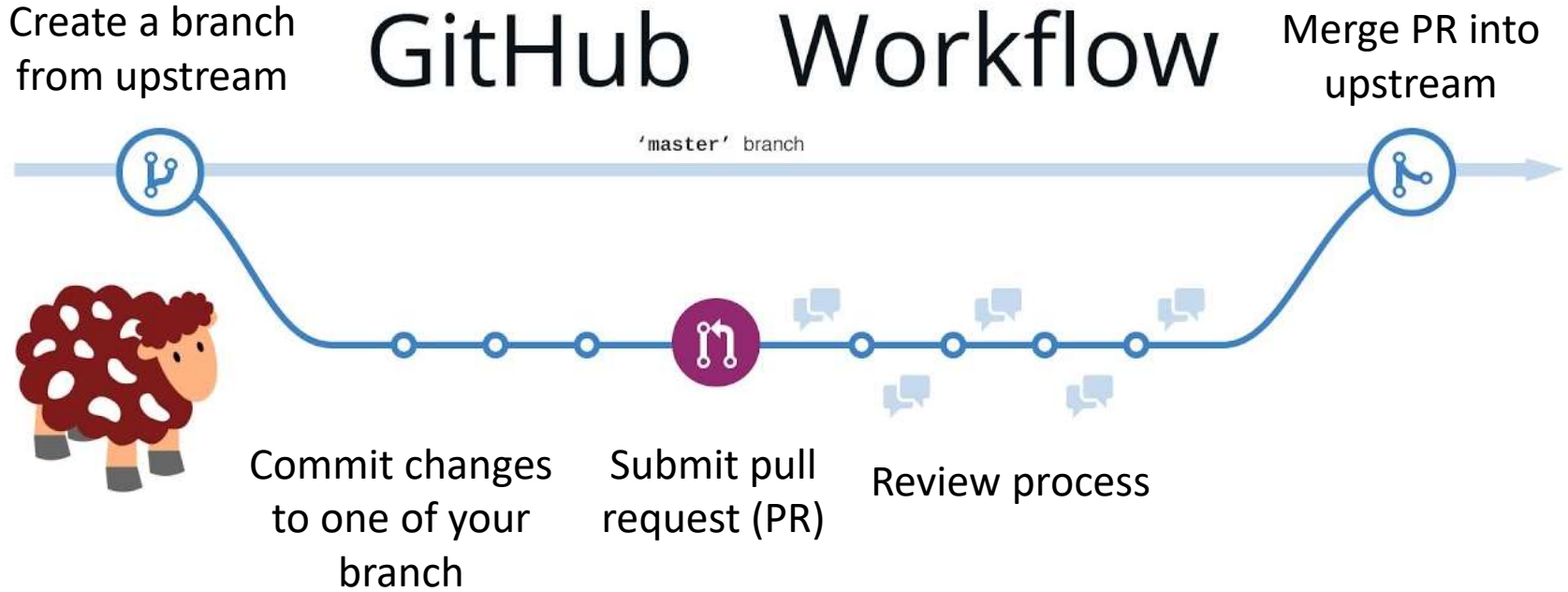


What is github?

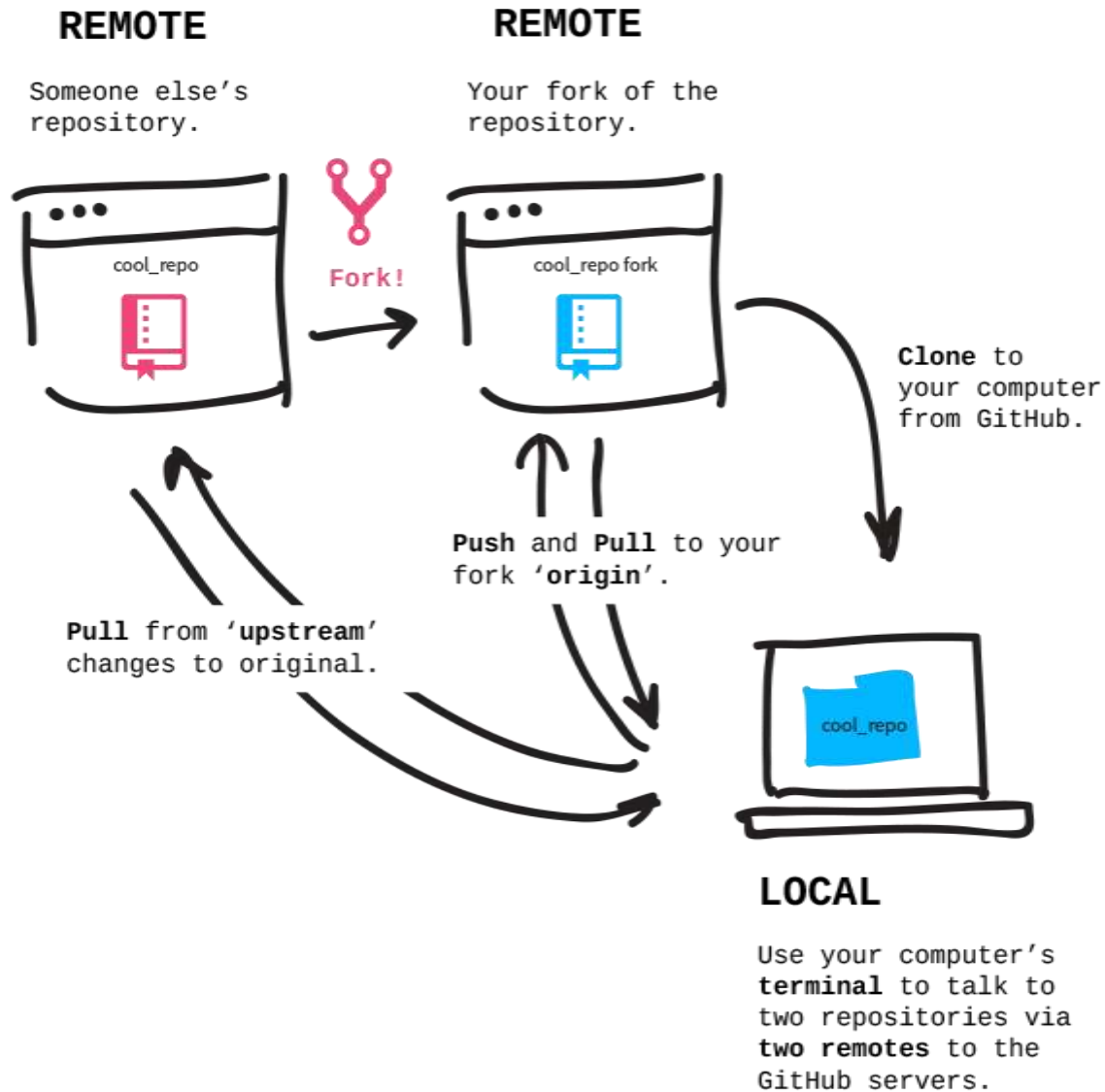
- GitHub is a git repository hosting service with its own features
 - Web-based graphical interface
 - provides a centralised place where people discuss the changes
 - “Social coding”
 - Open discussion in the issue tracker or PR submission, wiki, etc



How to use github?



How to use github?



Contribute to an open-source project before git/github

1. manually download the project's source code
2. make your changes locally
3. create a list of changes called a 'patch' and then e-mail the patch to the project's maintainer
4. The maintainer would then have to evaluate this patch, possibly sent by a total stranger and decide whether to merge the changes.

Tedious and not manageable

Why is github so useful/popular?

github web interface makes things easier

- Share code with other developers and the public
- Manage issues
- Manage pull request (code comparison and review)
- Maintain code

The screenshot shows a GitHub pull request (PR) titled "Fix tests and tidy up CI #2065". The PR is merged and was created by francisco-dlp on 18 Oct. The PR description states: "Travis and appveyor were failing because of a few reasons; This PR fixes it, removes a few warnings generated during the tests and also tidies up CI." The progress of the PR is listed with several items, all of which are checked off, indicating they have been completed. The PR is labeled with "affects: tests" and "type: bug-fix". The PR is reviewed by sem-geologist on 10 Oct. The code diff shows changes to the file hyperspy/misc/io/fei_stream_readers.py, specifically adding a try block and importing sparse.

Fix tests and tidy up CI #2065 Edit

Merged francisco-dlp merged 12 commits into hyperspy:RELEASE_next_patch from ericpre:fix_cleanup_decorator_plot_testing on 18 Oct

Conversation 30 Commits 12 Checks 0 Files changed 10 +60 -96

ericpre commented on 30 Sep • edited • Member

Description of the change

Travis and appveyor were failing because of a few reasons; This PR fixes it, removes a few warnings generated during the tests and also tidies up CI.

Progress of the PR

- Fix decorator issue with matplotlib 3.0 (I could not find a way to use the public API to do this);
- matplotlib 3.0 fixes a bug in the layout, so the baseline image needs to be update;
- set requirements to matplotlib == 3.0 for testings only;
- pin matplotlib to 2.2.3 for testing.
- fix nusb issue when creating array from empty list and remove requirement nusb < 0.39;
- sparse is not an optional dependency, tidy up code accordingly;
- fix a plotting warning in the tests of the spikes removal tool;
- fix a warning during reading tests of protochips files;
- appveyor: install dependencies from conda-forge channel to be consistent with the installation of hyperspy with conda (and also travis);
- ready for review.

Labels: affects: tests, type: bug-fix

Projects: None yet

Milestones: v1.4.1

Notifications: Unsubscribe

3 participants

sem-geologist reviewed on 10 Oct

```

hyperspy/misc/io/fei_stream_readers.py
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```

sem-geologist on 10 Oct • edited • Contributor

so sparse is going to be hard dependency ?

Why is github so useful/popular?

github web interface makes things easier

- Review and discuss changes during pull request (PR) review

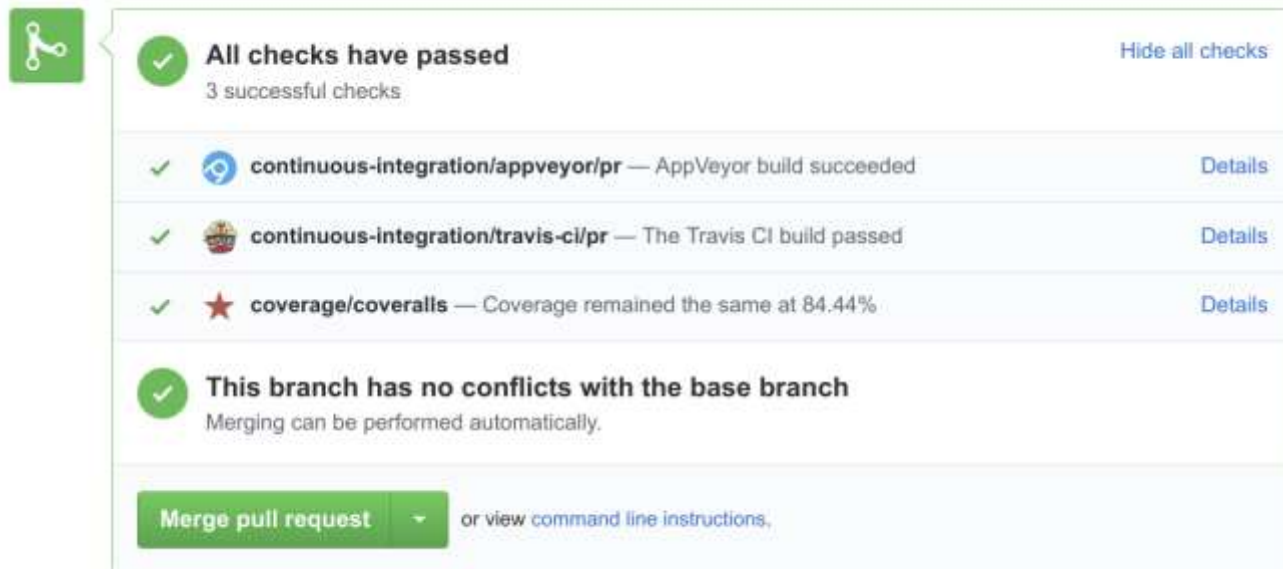
The screenshot displays a GitHub pull request interface. On the left, a diff view shows changes to a file named `install.py`. The changes are highlighted in alternating red and green blocks. The original code (left) includes a list of dependencies in the `DEPS` variable and a `conda install` command. The proposed changes (right) add `sparse` and `mamba` to the dependencies and update the `conda install` command to use `conda-forge`.

On the right side of the interface, a discussion thread is visible. It contains five messages from users `francisco-dlp` and `ericpre`, dated 18 Oct. The messages discuss the rationale for using `conda-forge` instead of the standard `anaconda` repository and the removal of the `test` optional dependency.

At the bottom of the discussion thread, there is a `Reply...` input field and a `Resolve conversation` button.

Why is github so useful/popular?

- Continuous integration
 - For each PR, the code is tested automatically against a suite of tests using external services (Github Actions, Azure, etc.)
 - ~4220 *unit tests* continuously checking that no regression is introduced by new changes



The screenshot displays a GitHub pull request status. At the top, a green checkmark icon is followed by the text "All checks have passed" and "3 successful checks". To the right of this text is a link that says "Hide all checks". Below this, there are three individual check items, each with a green checkmark and a "Details" link:

- continuous-integration/appveyor/pr — AppVeyor build succeeded
- continuous-integration/travis-ci/pr — The Travis CI build passed
- coverage/coveralls — Coverage remained the same at 84.44%

Below these items, there is a green checkmark icon followed by the text "This branch has no conflicts with the base branch" and "Merging can be performed automatically." At the bottom, there is a green button that says "Merge pull request" and a link that says "or view command line instructions."

HyperSpy developer guide

DEVELOPER GUIDE

☐ Introduction

Getting started

1. Start using HyperSpy and understand it

2. Got a problem? – ask!

3. Contribute – yes you can!

4. Contributing code

Using Git and GitHub

Running and writing tests

Writing documentation

Coding style

Tips for writing methods that work on lazy signals

Speeding up code

Writing packages that extend HyperSpy

Useful information

API REFERENCES

hyperspy

CREDITS AND CITATION

Credits

Citing HyperSpy

📖 Read the Docs

v: stable ▾

3. Contribute – yes you can!

You don't need to be a professional programmer to contribute to HyperSpy. Indeed, there are many ways to contribute:

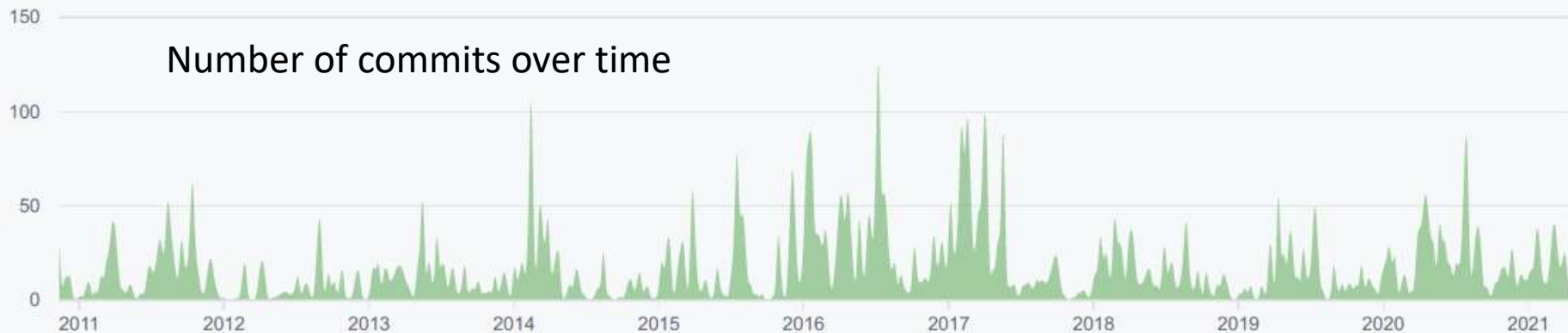
1. Just by asking a question in our [Gitter chat room](#) instead of sending a private email to the developers you are contributing to HyperSpy. Once you get more familiar with HyperSpy, it will be awesome if you could help others with their questions.
2. Issues reported in the [issues tracker](#) are precious contributions.
3. [Pull request](#) reviews are essential for the sustainability of open development software projects and HyperSpy is no exception. Therefore, reviews are highly appreciated. While you may need a good familiarity with the HyperSpy code base to review complex contributions, you can start by reviewing simpler ones such as documentation contributions or simple bug fixes.
4. Last but not least, you can contribute code in the form of documentation, bug fixes, enhancements or new features. That is the main topic of the rest of this guide.

4. Contributing code

You may have a very clear idea of what you want to contribute, but if you're not sure where to start, you can always look through the issues and pull requests on the [GitHub Page](#). You'll find that there are many known areas for development in the issues and a number of pull-requests are partially finished projects just sitting there waiting for a keen new contributor to come and learn by finishing.

HyperSpy community

- Code contributors
 - ~49 contributors in total from many different labs
 - A few contributors change jobs
 - Their github profile may have been useful for their successful application
 - ~ 20 of them are a one off contribution

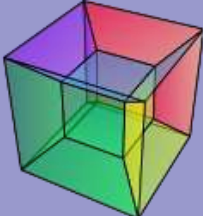


- Many more people following the gitter chat
 - Bug report, user feedback, requests, etc.

The HyperSpy eco-system last year

- Extension registration: other libraries can create their **specific Signal**

EELS Machine learning
Big data
Multi-dimensional
Visualisation and interactivity



EDS
IO
holography
Curve-fitting

HyperSpy-ipywidget

HyperSpy-traitsui

HyperSpyUI

cathodoluminescence
LumiSpy
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Particles analysis

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Atomic position fitting
Quantitative STEM
Atomap
Strain mapping

4D STEM
Magnetic measurement
pixStem
Differential contrast imaging

Strain mapping
Electron cristallography
pyXem
Orientation mapping
Scanning Electron diffraction

Electron Correlation Microscopy
Angular Correlations
EMpyer
Fluctuation Electron Microscopy

Other extension to come

The HyperSpy eco-system as of today

- Extension registration: other libraries can create their **specific Signal**

EELS Machine learning
Big data EDS
Multi-dimensional IO
Visualisation and interactivity holography
Curve-fitting

HyperSpy-ipywidget

HyperSpy-traitsui

HyperSpyUI

Atomic position fitting
Quantitative STEM
Atomap
Strain mapping

Differential contrast imaging
Electron cristallography
Pair distribution function
pyXem
Scanning Electron diffraction
4D STEM

Other extension to come

cathodoluminescence
LumiSpy
photoluminescence

EBSD
Strain mapping
Kikuchipy
Orientation mapping

inpainting
inpystem
reconstruction techniques

segmentation
ParticleSpy
Particles analysis

pyMatchSeries
Non-rigid image registration

hyperspy_swift_library
Access nionswift libraries

pgure-svt
Denoising time-resolved microscopy

Future HyperSpy ecosystem and other relevant libraries

HyperSpyUI

HyperSpy-ipywidget

HyperSpy-traitsui

HyperSpy extension

HyperSpy aware library

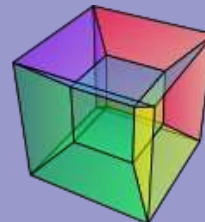
EELS

IO

EDS

Holography

Multi-dimensional
Visualisation and interactivity
Big data
Machine learning



Curve-fitting

pycroscopy

GMS 3

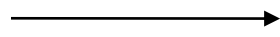
LiberTEM

tomviz

Nionswift

Python libraries for 4D STEM data analysis

- pyXem
- pixstem
- EMpyer
- py4DSTEM
- pycroscopy
- stemtools
- Various nionswift plugins
- LiberTEM
- ...



Optimised for high throughput on small computer clusters

All these open source libraries are doing **very similarly things**

Common issues with research software development

- Many publications present interesting data analysis workflow or methodological development
- These are **generally not easily accessible**
 - proprietary licence
 - not easily to install or to run (platform dependent, etc.)
 - not supported/up to date anymore
- May be **difficult to maintain** for the developer
- Implementation need to be generic and robust
- Rely on a specific research group (most of the time by one or a few PhD student or a post-doc..)
 - Not sustainable

Package distribution

- Integration with other libraries and workflow
- Installation needs to be easy

- Install Python 3.7 from [Anaconda](#)
- Open an Anaconda Prompt Terminal and create a new environment by running:

```
1 conda create --name hyperspy_env python=3.7
```

- Activate the above environment by:

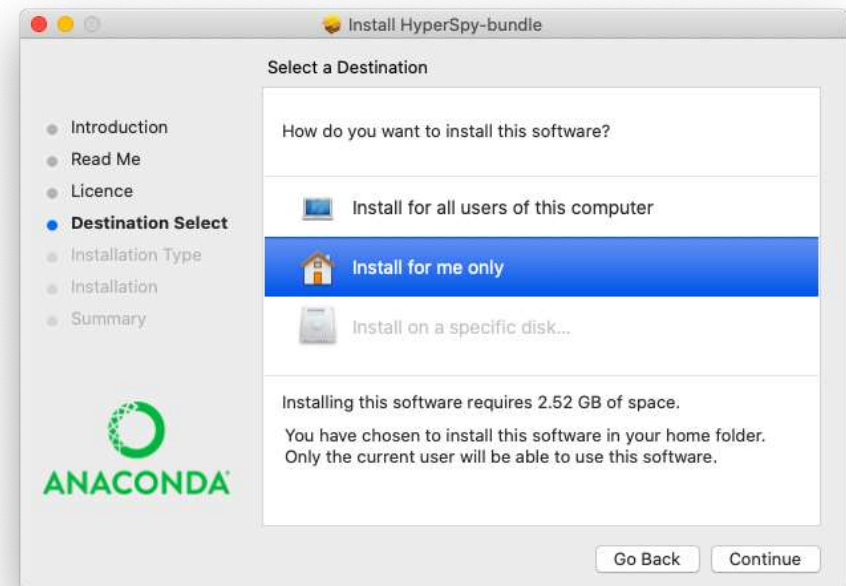
```
1 WINDOWS: activate hyperspy_env
2 LINUX, macOS: source activate hyperspy_env
```

- Install the packages by running the following commands:

```
1 conda install hyperspy -c conda-forge
2 jupyter labextension install @jupyter-widgets/jupyterlab-manager
3 conda install -c conda-forge pyxem
4 conda install -c conda-forge atomap
```

- Not straightforward for beginner
- Usually not valid anymore after some time

HyperSpy bundle installer



- For beginner (and advanced) users
- Expected to work out of the box
- Very similar to Anaconda/Miniconda but includes relevant libraries

What makes HyperSpy today?

- Use tools and development practises which have proven to be successful for open source project
- HyperSpy is supported by its own community
- HyperSpy doesn't rely on a specific research group/institution
- Peer-reviewed and open-source development
- HyperSpy is a mature library
 - API fairly stable
 - doesn't break as much as before
- HyperSpy can be integrated easily in other software
 - Framework for the development of other libraries
 - HyperSpy will be split in the near future
 - Better modularity
 - Easier, faster implementation of new features

Achievement of HyperSpy and its community

- HyperSpy managed to built a *distributed* community of users/contributor
 - Led by its own contributors
 - Decision based on contributors consensus
- Motivate (at least not discourage) users
 - Pay attention to users feedback
 - From user to contributor: make the learning curve easier
- What are contributors doing?
 - Contribution to user guide, tutorials and online discussion
 - Code writing and/or code review

This is one way to make a library
useful and sustainable

As individual is it worth contributing to HyperSpy?

- HyperSpy acknowledgement through zenodo DOI
 - One DOI for each release (important for reproducibility)
 - New contributors will be acknowledged
- Very good training
- Contribution to HyperSpy (or any other library) can be useful for career development
 - Github profile can be used as linkedin, etc.
 - Recognition by the community

As a group/organisation/company, why supporting HyperSpy?

- As PI/group leader
 - PI are not acknowledged but they can benefit a lot from the expertise gained through HyperSpy
 - Fairly useful “training” for post-doc/student
 - Remove dependence on expansive license for software or plugins
- Companies, conflict of interest?!
 - Some companies start to show interest in open source
 - Still a bit difficult: paradigm shift required
 - Customers are pushing enough to convince companies
 - Extend data processing capabilities of their software
 - By being compatible with open source software, companies can offer solution there could not afford otherwise